

# A Lower Bound for the Energy of Hypoenergetic and Non Hypoenergetic Graphs

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## Abstract

Let  $G$  be a simple undirected graph with  $n$  vertices and  $m$  edges. The energy of  $G$ ,  $\mathcal{E}(G)$  corresponds to the sum of its singular values. This work obtains lower bounds for  $\mathcal{E}(G)$  where one of them generalizes a lower bound obtained by Mc Clelland in 1971 to the case of graphs with given nullity. An extension to the bipartite case is given and, in this case, it is shown that the lower bound  $2\sqrt{m}$  is improved. The equality cases are characterized. Moreover, a simple lower bound that considers the number of edges and the diameter of  $G$  is derived. A simple lower bound, which improves the lower bound  $2\sqrt{n-1}$ , for the energy of trees with  $n$  vertices and diameter  $d$  is also obtained.

## 1 Notation and Preliminaries

In this work we deal with an  $(n, m)$ -graph  $G$  which is an undirected simple graph with vertex set  $V(G)$  and edge set  $E(G)$  of cardinality  $n$  and  $m$ , respectively. As usual we denote the adjacency matrix of  $G$  by  $A = A(G)$ . The eigenvalues of  $G$  are the eigenvalues

of  $A$  (see e.g. [5, 6]). Its eigenvalues will be denoted (and ordered) by  $\lambda_1 \geq \dots \geq \lambda_n$ . We denote the spectrum of a graph  $G$  by  $\sigma(G)$ . The singular values of  $G$  are the square roots of the eigenvalues of  $A^*A$ , where  $A^*$  is the conjugate transpose matrix of  $A$ . Since,  $A$  is real and symmetric the singular values of  $G$  are the absolute values of its eigenvalues. If  $G$  is a connected graph, then  $A(G)$  is a nonnegative irreducible matrix [5]. The complete graph, the cycle, with  $n$  vertices and the complete bipartite graph with bipartition  $(X, Y)$  are denoted by  $K_n, C_n$  and  $K_{x,y}$ , respectively, where the cardinals of  $X$  and  $Y$  are  $x$  and  $y$ . We recall now some concepts from Matrix Theory used throughout the text. In this paper  $R$  and  $M$  stands for a Hermitian complex and an arbitrary complex matrix, respectively, both of orders  $n$ . The *energy* of  $R$ , denoted by  $\mathcal{E}(R)$ , is the sum of its singular values that is, the sum of the absolute values of its eigenvalues. If  $R$  is a non-negative matrix, then  $R$  is symmetric and its spectral radius,  $\rho = \rho(R)$ , and its largest eigenvalue coincide, see [18].

The *nullity* of  $M$ , denoted by  $\eta(M)$ , corresponds to the multiplicity of the null eigenvalue of  $M^*M$ , where  $M^*$  is the conjugate transpose matrix of  $M$ . Thus, if  $M$  is nonsingular then  $\eta(M) = 0$ . For a graph  $G$ , the nullity of  $A(G)$  is called the *nullity* of  $G$  and it is denoted by  $\eta(G)$ , see [10]. Consequently, a graph  $G$  is called *nonsingular* if  $\eta(G) = 0$  otherwise,  $G$  is called *singular*. The *rank* of a square matrix  $M$  of order  $n$  is  $r(M) = n - \eta(M)$ , see [17]. When  $M = A(G)$  we simply denote  $r(A(G))$  by  $r$ . On the other hand, the *k-th elementary symmetric sum* of the eigenvalues  $\mu_1, \mu_2, \dots, \mu_n$  of a square matrix  $M$  of order  $n$ , see [17], is defined as

$$\Upsilon_k(M) = \sum_{1 \leq i_1 < i_2 < \dots < i_k \leq n} \mu_{i_1} \mu_{i_2} \dots \mu_{i_k}. \quad (1)$$

Note that  $\Upsilon_n(M) = \det(M)$  and  $\Upsilon_1(M) = \text{tr}(M)$ , with  $\text{tr}(\cdot)$  denoting the trace of a square matrix. For a matrix  $M$  of order  $n$ , let  $M[i_1, i_2, \dots, i_k]$  be the principal submatrix of  $M$  whose  $j$ -th row and column are labeled by  $i_j$ , for  $1 \leq j \leq k$ . Then,  $\det(M[i_1, i_2, \dots, i_k])$  is a *principal minor of order k of M* and it is denoted by  $\Delta_M(i_1, i_2, \dots, i_k)$ . A well-known result of linear algebra is [17] :

**Lemma 1.** [17] *Let  $M$  be a matrix of order  $n$  and let  $p(\mu) = \det(\mu I - M)$ , where,  $I$  denotes the identity matrix. Let*

$$p(\mu) = \lambda^n + c_1\mu^{n-1} + c_2\mu^{n-2} + \dots + c_{n-1}\mu + c_n = 0.$$

*If  $\Upsilon_k(M)$  is the k-th symmetric function of the eigenvalues  $\mu_1, \mu_2, \dots, \mu_n$  of  $M$ , then*

1.  $c_k = (-1)^k \sum (\text{all } k \times k \text{ principal minors})$ ;
2.  $\Upsilon_k(M) = \sum (\text{all } k \times k \text{ principal minors})$ ;
3.  $\text{tr}(M) = \mu_1 + \mu_2 + \cdots + \mu_n = -c_1$ ;
4.  $\det(M) = \mu_1 \mu_2 \cdots \mu_n = (-1)^n c_n$ .

Therefore,

$$|c_k| = |\Upsilon_k(M)| = \left| \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq n} \Delta_M(i_1, i_2, \dots, i_k) \right|. \quad (2)$$

**Remark 1.** Let  $R$  be a Hermitian of rank  $n-\kappa$  whose nonzero eigenvalues are  $\alpha_{j_1}, \dots, \alpha_{j_{n-\kappa}}$ , then

$$\left| \sum_{1 \leq i_1 < i_2 < \cdots < i_{n-\kappa} \leq n} \Delta_R(i_1, i_2, \dots, i_{n-\kappa}) \right| = \left| \prod_{l=1}^{n-\kappa} \alpha_{j_l} \right| = |\Upsilon_{n-\kappa}(R)|.$$

The Frobenius matrix norm of a square complex matrix  $M$ , denoted by  $|M|$ , is defined as the square root of the sum of the squares of its singular values. In consequence, if  $R$  is a Hermitian matrix of order  $n$  with eigenvalues  $\alpha_1, \alpha_2, \dots, \alpha_n$ ,

$$|R|^2 = \sum_{i=1}^n |\alpha_i|^2.$$

The paper is organized as follows. At Section 2 the definition of energy of a graph is recalled and known lower bounds for  $\mathcal{E}(G)$  and the main results without proof are introduced.

At Section 3, the proofs of the results introduced in the previous section are done. In particular, some lower bounds for  $\mathcal{E}(G)$  are given where one of them generalizes a lower bound obtained by Mc Clelland in 1971 to the case of graphs with given nullity. An extension to the bipartite case is given and, in this case, it is shown that the lower bound  $2\sqrt{m}$  introduced by Caporossi et al. in [4] is improved. The equality cases are characterized. Moreover, a simple lower bound that considers the number of edges and the diameter of  $G$  is derived. A simple lower bound, which improves the lower bound  $2\sqrt{n-1}$ , for the energy of trees with  $n$  vertices and diameter  $d$  is obtained. Additionally, at Section 4 some tables, comparing the results, are presented.

## 2 Motivation and the main results

The concept of energy of a graph appeared in Mathematical Chemistry and we briefly refer in this section its importance. The reader should refer to [12,14] (and the references therein) where more details can be found.

Therefore, for a graph  $G$ , the expression in Eq. (3)

$$\mathcal{E}(G) = \sum_{i=1}^n |\lambda_i|, \quad (3)$$

where  $\lambda_1, \dots, \lambda_n$  are the eigenvalues of the graph, is called the *energy* of the graph  $G$ , ([11]). It is worth to be mentioned that in the recent literature this graph invariant has been extensively studied, namely the search for its upper bounds. Concerning lower bounds for the energy of a graph the reader should be referred, for instance, to [1–3,15,20]. For an arbitrary graph  $G$ , in [16] McClelland's obtained the following lower bound for  $\mathcal{E}(G)$ :

$$\mathcal{E}(G) \geq \sqrt{2m + n(n-1) |\det(A)|^{2/n}}. \quad (4)$$

where  $\det(A)$  denotes the determinant of the matrix  $A = A(G)$ . A lower bound for the energy of a graph in terms of the number of vertices, edges and determinant of the adjacency matrix that, under certain conditions improved the classical McClelland's lower bound can be seen in [7,8].

The following simple lower bound for a graph  $G$  with  $m$  edges was introduced by Caporossi et al. in [4] and the equality case was discussed. In fact,

$$\mathcal{E}(G) \geq 2\sqrt{m}, \quad (5)$$

with equality if and only if  $G$  consists of a complete bipartite graph  $K_{a,b}$  such that  $ab = m$  and arbitrarily many isolated vertices. A lower bound for the energy of symmetric matrices and graphs was introduced in [1]. A spectral lower bound for the energy can be seen in [4], following directly from the fact that  $\text{tr}(A(G)) = 0$  and it is:

$$\mathcal{E}(G) \geq 2\lambda_1, \quad (6)$$

where, if  $G$  is connected, the equality holds in (6), for example, if  $G$  is a complete graph and a complete bipartite graph.

Next we present the results of this work. Their proofs are presented at Section 3. The following theorem generalizes the lower bound in (4) for Hermitian matrices  $R$ , such that  $\eta(R) = \kappa$ . Some equality cases are discussed.

**Theorem 2.** *Let  $R$  be a Hermitian matrix with nullity  $\eta(R) = \kappa$ , where  $0 \leq \kappa \leq n - 1$ . Then*

$$\mathcal{E}(R) \geq \frac{\sqrt{4|R|^2 + (2(n - \kappa) - 1)^2 - 1) |\Upsilon_{n-\kappa}(R)|^{\frac{2}{n-\kappa}}}{2}. \quad (7)$$

*The equality holds in (7) if and only if the nonzero eigenvalues of  $R$  have the same absolute value. Moreover, if  $R$  is a nonnegative irreducible matrix the equality holds if and only if  $R$  is permutationally equivalent to a block matrix of the form,*

$$\begin{pmatrix} 0 & S \\ S^T & 0 \end{pmatrix} \quad (8)$$

*where  $\kappa = n - 2$  and  $S$  is a rank one matrix.*

**Remark 2.** *Note that the list of eigenvalues of a matrix  $R$  can be unknown and, therefore, its not possible to calculate directly the energy of  $R$ . However, knowing  $\Upsilon_{n-\kappa}(R)$ , and one way to obtain it without knowing the eigenvalues is calculating  $c_{n-\kappa}$ , the coefficient of  $x^\kappa$  of the characteristic polynomial of  $R$ , with the formula in (7) one can approximate the energy. If  $R$  is the adjacency matrix of a graph  $G$  the expression can be obtained by a result in [5] which obtains the coefficients of the characteristic polynomial in terms of the so called “elementary figures”.*

## 2.1 Results for general graphs

In this subsection the results for general graphs are presented. In order to proceed, and to simplify the notation, sometimes we will set  $n - \kappa = r$  and, for any graph  $G$ ,  $\Upsilon_r(G) = \Upsilon_r(A(G))$ .

Note that, if in Theorem 2 the Hermitian matrix  $R$  is replaced by the adjacency matrix of a graph  $G$  the inequality (9) in Theorem 3 below is obtained. The proof of the inequality in (10) is given in Section 3.

**Theorem 3.** *Let  $G$  be an  $(n, m)$ -graph without isolated vertices, with nullity  $\eta(G) = \kappa = n - r$ , where  $0 \leq \kappa \leq n - 1$  ( $1 \leq r \leq n$ ). Then*

1.

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4r(r-1)} |\Upsilon_r(G)|^{\frac{2}{r}}}{2}. \quad (9)$$

2.

$$\mathcal{E}(G) \geq r |\Upsilon_r(G)|^{\frac{1}{r}}. \quad (10)$$

The equalities hold in (9) and in (10) if and only if the nonzero eigenvalues of  $G$  have the same absolute value. Note that if  $G$  is connected the equality holds if and only if  $G = K_{a,b}$  the complete bipartite graph, with  $a + b = \kappa + 2$ . Otherwise  $G = \cup_{j=1}^{\ell} K_{a_j, b_j}$ , with  $a_j b_j = a_i b_i$ , for  $i \neq j$ ,  $\ell = \frac{n-\kappa}{2}$  and  $n = \sum_{j=1}^{\ell} (a_j + b_j)$ .

**Remark 3.** Recalling the equation in (2) one can see that  $|\Upsilon_r(G)|$  corresponds to  $|c_r|$ . Since all the entries of  $A(G)$  are integers, from item 1. in Lemma 1, and taking into account that it is considered the absolute value of the product of the nonzero eigenvalues of  $G$ , it follows that the coefficient  $c_r$  is a nonzero integer. In consequence,

$$|\Upsilon_r(G)| \geq 1, \quad \forall 1 \leq r \leq n. \quad (11)$$

**Remark 4.** Recalling that a graph  $G$  is called hypoenergetic if its energy is less than the number of vertices of  $G$ , see [14]. The inequalities in (10) and (11) show directly a known result, namely, that if  $\eta(G) = 0$  then  $G$  is not hypoenergetic. This remark will be referred in the last section of conclusions.

From inequalities (9) and (11), we derive the following result.

**Corollary 4.** Let  $G$  be an  $(n, m)$ -graph without isolated vertices, with nullity  $\eta(G) = \kappa = n - r$  with  $0 \leq \kappa \leq n - 1$  ( $1 \leq r \leq n$ ). Then

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4r(r-1)}}{2}. \quad (12)$$

The equality holds in (12) if and only if  $G = K_2$ .

**Remark 5.** If  $r(r-1) > 2m$ , for example, for  $G = C_n$ , see [10], then the lower bound in (12) improves the lower bound in (5).

Recall that the *diameter* of a connected graph  $G$ , denoted by  $\text{diam}(G)$ , is the maximum distance between two vertices of  $G$ .

In [6, Theorem 3.3.5] it was proven that if  $G$  is a connected graph with precisely  $\beta$  distinct eigenvalues then

$$\text{diam}(G) + 1 \leq \beta. \quad (13)$$

Taking into account Theorem 3 and the inequality in (13) the following results are obtained.

**Corollary 5.** *Let  $G$  be an  $(n, m)$  connected graph, with nullity  $\eta(G) = \kappa$ , where  $0 \leq \kappa \leq n - 1$ . Then*

1. *If  $\kappa > 0$  then*

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4\text{diam}(G)(\text{diam}(G) - 1) |\Upsilon_{n-\kappa}(G)|^{\frac{2}{n-\kappa}}}}{2}, \quad (14)$$

2. *If  $\kappa = 0$ , then*

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4\text{diam}(G)(\text{diam}(G) + 1) |\det(A(G))|^{\frac{2}{n}}}}{2}. \quad (15)$$

Taking into account Corollary 5 and (11) the next corollary is obtained.

**Corollary 6.** *Let  $G$  be an  $(n, m)$  connected graph, with nullity  $\eta(G) = \kappa$ , where  $0 \leq \kappa \leq n - 1$ . Then*

1. *If  $\kappa > 0$ , then*

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4\text{diam}(G)(\text{diam}(G) - 1)}}{2}, \quad (16)$$

2. *If  $\kappa = 0$ , then*

$$\mathcal{E}(G) \geq \frac{\sqrt{8m + 4\text{diam}(G)(\text{diam}(G) + 1)}}{2}. \quad (17)$$

## 2.2 Results for bipartite and tree graphs

In this subsection the results valid for bipartite graphs and trees are presented. Recall that  $r = n - \kappa$ .

**Theorem 7.** Let  $G$  be an  $(n, m)$  bipartite graph without isolated vertices, with  $\eta(G) = \kappa = n - r$ , where  $0 \leq \kappa \leq n - 1$  ( $1 \leq r \leq n$ ). Then

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4r(r-2)} |\Upsilon_r(G)|^{\frac{2}{r}}}{2}. \quad (18)$$

with equality if and only if all the nonzero eigenvalues of  $G$  have the same absolute value in other words, if and only if  $G = \cup_{j=1}^{\ell} K_{a_j, b_j}$ , with  $a_j b_j = a_i b_i$ , for  $i \neq j$ ,  $\ell = \frac{n-\kappa}{2}$  and  $n = \sum_{j=1}^{\ell} (a_j + b_j)$ .

Taking into account Theorem 7 and inequality in (11), we obtain

**Corollary 8.** Let  $G$  be an  $(n, m)$  bipartite graph without isolated vertices, with  $\eta(G) = \kappa = n - r$ , where  $0 \leq \kappa \leq n - 1$  ( $1 \leq r \leq n$ ). Then

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4r(r-2)}}{2}. \quad (19)$$

**Remark 6.** If  $r = n - \kappa > 2$ , then the lower bound in (19) improves the lower bound in (5).

Attending to Theorem 7 and inequality in (13), the next corollary follows.

**Corollary 9.** Let  $G$  be an  $(n, m)$  connected bipartite graph, with nullity  $\eta(G) = \kappa$ , where  $0 \leq \kappa \leq n - 1$ .

1. If  $\kappa > 0$ , then

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4\text{diam}(G)(\text{diam}(G) - 2)} |\Upsilon_{n-\kappa}(G)|^{\frac{2}{n-\kappa}}}{2}, \quad (20)$$

2. If  $\kappa = 0$ , then

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4(\text{diam}(G)^2 - 1)} |\det(A(G))|^{\frac{2}{n}}}{2}. \quad (21)$$

Taking into account Corollary 9 and (11) the next corollary is obtained.

**Corollary 10.** Let  $G$  be an  $(n, m)$  bipartite connected graph, with nullity  $\eta(G) = \kappa$ , where  $0 \leq \kappa \leq n - 1$ .

1. If  $\kappa > 0$ , then

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4\text{diam}(G)(\text{diam}(G) - 2)}}{2}, \quad (22)$$



2. If  $\kappa = 0$ , then

$$\mathcal{E}(G) \geq \frac{\sqrt{16m + 4(\text{diam}(G)^2 - 1)}}{2}, \quad (23)$$

3. In particular, if  $G$  is a tree of diameter  $d$ , and nullity  $\kappa > 0$ , then

$$\mathcal{E}(G) \geq \sqrt{4(n-1) + d^2 - 2d}. \quad (24)$$

**Remark 7.** Since the rank of a bipartite graph is an even number all the trees with an odd number of vertices have nullity  $\kappa > 0$ . In consequence, the inequality in (24) holds for this type of trees.

### 3 Proof of the main results

In this section the proofs of Theorems 2 and 7 and Corollaries 5 and 9 described at Section 2 are presented.

*Proof. of Theorem 2* Let  $\alpha_{j_1} \geq \alpha_{j_2} \geq \dots \geq \alpha_{j_{n-\kappa}}$  be the nonzero eigenvalues of  $R$ . It is clear that

$$\mathcal{E}(R) = |\alpha_{j_1}| + |\alpha_{j_2}| + \dots + |\alpha_{j_{n-\kappa}}|.$$

Thus

$$\begin{aligned} \mathcal{E}(R)^2 &= (|\alpha_{j_1}| + |\alpha_{j_2}| + \dots + |\alpha_{j_{n-\kappa}}|)^2 \\ &= \sum_{\ell=1}^{n-\kappa} |\alpha_{j_\ell}|^2 + \sum_{\ell_1 \neq \ell_2} |\alpha_{j_{\ell_1}}| |\alpha_{j_{\ell_2}}|. \end{aligned}$$

Since the geometric mean of a set of positive numbers is not greater than the arithmetic mean, and the equality holds if and only if all of them are equal, we have:

$$\begin{aligned} \sum_{\ell_1 \neq \ell_2} |\alpha_{j_{\ell_1}}| |\alpha_{j_{\ell_2}}| &\geq r(r-1) \left( \prod_{\ell_1 \neq \ell_2} |\alpha_{j_{\ell_1}}| |\alpha_{j_{\ell_2}}| \right)^{\frac{1}{r(r-1)}} \\ &= r(r-1) |\Upsilon_r(R)|^{\frac{2}{r}}. \end{aligned}$$

Then the form given in (7) is obtained from the inequality

$$\mathcal{E}(R) \geq \sqrt{|R|^2 + r(r-1) |\Upsilon_r(R)|^{\frac{2}{r}}}. \quad (25)$$

Finally, the equality holds if and only if

$$|\alpha_{j_1}| = |\alpha_{j_2}| = \dots = |\alpha_{j_r}|. \quad (26)$$

From (26), attending to the definition of imprimitivity  $h$  in [18, Section III], we have  $h = n - \kappa$ . Additionally, if  $R$  is nonnegative irreducible and symmetric, its imprimitivity index must be  $h = 2$ . Therefore  $\kappa = n - 2$ . Moreover  $R$  is cogredient (that is, permutationally similar), to a matrix of the form in (8) and as  $\kappa = n - 2$ , the block  $S$  is a rank one matrix. By [18, Theorem 4.2] it is clear that, in this case,  $\rho(R)$ , (the spectral radius of  $R$ ), and  $-\rho(R)$  are the only nonzero eigenvalues of  $R$ . The proof of the inequality in (10) is a direct application of the geometric-arithmetic mean of a set of positive numbers and its equality case.  $\square$

Note that the inequality in (25) is the inequality in (4) whenever  $\kappa = 0$ . Moreover, By the equality in (2), the term  $|\Upsilon_r(R)|^{\frac{2}{r}}$  is a matrix invariant that can be replaced, for instance, by  $\det(R)$ .

**Proof. of the inequality in (10)** The proof of the inequality in (10) is a direct application of the geometric-arithmetic mean on a set of  $r$  positive numbers and its equality case.  $\square$

**Proof. of Corollary 5** If  $\lambda_{i_1}, \dots, \lambda_{i_\beta}$  are the distinct eigenvalues of  $G$  and  $\kappa \geq 1$ , then there is only one eigenvalue, say  $\lambda_{i_\ell}$  such that  $\lambda_{i_\ell} = 0$  and we have  $r = n - \kappa \geq \beta - 1 \geq \text{diam}(G) + 1 - 1 = \text{diam}(G)$ . On the contrary case, if  $\kappa = 0$  we have  $r = n - \kappa = n \geq \beta \geq \text{diam}(G) + 1$ .  $\square$

**Proof. of Theorem 7** Since  $\lambda \in \sigma(G) - \{0\}$  if only if  $-\lambda \in \sigma(G) - \{0\}$ , there exists an integer  $t$  such tha  $n - \kappa = 2t$ . Moreover

$$\mathcal{E}(G) = 2 \sum_{\ell=1}^t |\lambda_{i_\ell}|.$$

In consequence,

$$\begin{aligned} \mathcal{E}(G)^2 &= 4 \left( \sum_{\ell=1}^t |\lambda_{i_\ell}| \right)^2 = 4 \left[ \sum_{\ell=1}^t |\lambda_{i_\ell}|^2 + 2 \sum_{1 \leq \ell_1 < \ell_2 \leq t} |\lambda_{i_{\ell_1}}| |\lambda_{i_{\ell_2}}| \right] \\ &\geq 4 \left[ \sum_{\ell=1}^t |\lambda_{i_\ell}|^2 + t(t-1) \left( \prod_{\ell=1}^t |\lambda_{i_\ell}|^{t-1} \right)^{\frac{2}{t(t-1)}} \right] \\ &= 4m + (n - \kappa)(n - \kappa - 2) |\Upsilon_{n-\kappa}(G)|^{\frac{2}{n-\kappa}}. \end{aligned}$$

The equality holds if and only if all the nonzero eigenvalues of  $G$  have the same absolute value. In order to simplify the notation we write  $\Gamma = |\Upsilon_{n-\kappa}(G)|^{\frac{2}{n-\kappa}}$ . Therefore, the

previous inequality is equivalent to:

$$(n - \kappa)^2 \Gamma - 2(n - \kappa) \Gamma + 4m - \mathcal{E}(G)^2 \leq 0.$$

Reading the latter inequality as a quadratic inequality in the variable  $n - \kappa$ , we obtain

$$\frac{\sqrt{16m + ((2(n - \kappa) - 2)^2 - 4) \Gamma}}{2} \leq \mathcal{E}(G),$$

which (except by an algebraic step) proves (18).  $\square$

## 4 Computational experiments

Next some comparatives examples for different values of  $n$  are presented.

Using different graphs the lower bounds in the paper are compared. In order to control the differences among the lower bound (4) and the new lower bound in (9) the rank  $r$  is given. The energies  $E$  and the lower bounds in (5), (6), (9), (10) and (12), are compared. Only the last 3 columns are the lower bounds found in the present work. We begin with  $n = 3$ :

Adjacency	$E$	$r$	(5)	(6)	(9)	(10)	(12)
$K_{1,2}$	2.8284	2	2.8284	2.8284	2.8284	2.8284	2.4495
$K_3$	4	3	3.7798	4	3.9401	3.7798	3.4641

$n = 4$ :

Adjacency	$E$	$r$	(5)	(6)	(9)	(10)	(12)
$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	4.4721	4	3.4641	3.2361	4.2426	4.0000	4.2426
$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$	4	2	4	4	4	4	3.1623
$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	4	3	3.4641	4	3.9401	3.7798	3.4641

$n = 5$  :

Adjacency	$E$	$r$	(5)	(6)	(9)	(10)	(12)
$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix}$	5.6272	4	4.4721	4.6858	5.1933	4.7568	4.6904
$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix}$	5.4641	4	4	3.4641	5.3651	5.2643	4.4721
$\begin{pmatrix} 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$	5.5959	4	4.4721	4.2716	5.1933	4.7568	4.6904

## 5 Conclusions

In order to conclude this work we would like to refer the importance of the study of these subjects. By one hand, some results on literature for instance, the authors in [9] say that “in general the rank of the adjacency matrix of a graph can be computed in polynomial time but we do not have a simple combinatorial expression for it”. The authors in [10] claim that “the nullity of a molecular graph has a far-reaching inference on the expected stability of unsaturated conjugated hydrocarbons”. On the other hand the definition of hypoenergetic graphs, (see [14]), suggests that there are many graphs (chemical or not) with nullity greater than zero as following Remark 4, one can say that hypoenergetic graphs with nullity zero do not exist. Another thing that justifies the present study is that many chemical trees have 0 as an eigenvalue, see, for instance, [13, 19]. Moreover, in this work, a new lower bound for the energy of non-singular graphs and some properties of the lower bound in (4) are recalled and studied. Additionally, for the bipartite case the lower bounds given in this work improve the known lower bound in (5) in both cases that is, they are valid for graphs with zero or non zero nullity. We also believe that the relation between the nullity of a graph and its energy deserves to be studied.

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## References

- [1] E. Andrade, M. Robbiano, B. San Martín, A lower bound for the energy of symmetric matrices and graphs, *Lin. Algebra Appl.* **513** (2017) 264–275.
- [2] N. Agudelo, J. Rada, Lower bounds of Nikiforov’s energy over digraphs, *Lin. Algebra Appl.* **494** (2016) 156–164.
- [3] Ş. B. Bozkurt Altındağ, D. Bozkurt, Lower bounds for the energy of (bipartite) graphs, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 9–14.
- [4] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs, 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996.
- [5] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs Theory and Applications*, Academic Press, New York, 1980.
- [6] D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.
- [7] K. Das, S.A. Mojallal, I. Gutman, Improving McClelland’s lower bound for energy, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 663–668.
- [8] I. Gutman, Bounds for total  $\pi$ -electron energy, *Chem. Phys. Lett.* **24** (1974) 283–285.
- [9] C. Godsil, G. Royle, *Algebraic Graph Theory*, Springer, New York, 2001.
- [10] I. Gutman, B. Borovićanin, Nullity of graphs: An updated survey, in: D. Cvetković, I. Gutman (Eds.), *Selected Topics on Applications of Graph Spectra*, Math. Inst., Belgrade, 2011, pp. 137–154.

- [11] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.) *Algebraic Combinatorics and Applications*, Springer, Berlin, 2001, 196–211.
- [12] I. Gutman, B. Furtula, The total  $\pi$ -electron energy saga, *Croat. Chem. Acta* **90** (2017) 359–368.
- [13] C. Heuberger, S. G. Wagner, Chemical trees minimizing energy and Hosoya index, *J. Math. Chem.* **46** (2009) 214–230.
- [14] X. Li, Y. Shi, I. Gutman *Graph Energy*, Springer, New York, 2012.
- [15] C. A. Marin, J. Monsalve, J. Rada, Maximum and minimum energy trees with two and three branched vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 285–306.
- [16] B.J. McClelland, Properties of the latent roots of a matrix: The estimation of  $\pi$ -electron energies, *J. Chem. Phys.* **54** (1971) 640–643.
- [17] C. D. Meyer, *Matrix Analysis and Applied Linear Algebra*, SIAM, Philadelphia, 2000.
- [18] H. Minc, *Nonnegative Matrices*, Wiley, New York, 1988.
- [19] O. Rojo, M. Robbiano, An explicit formula for eigenvalues of Bethe trees and upper bounds on the largest eigenvalue of any tree, *Lin. Algebra Appl.* **427** (2007) 138–150.
- [20] T. Tian, W. Yan, S. Li, On the minimal energy of trees with a given number of vertices of odd degree, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 3–10.